

```

chain nodes :
7 8 9 10 16 17 18 19
ring nodes :
1 2 3 4 5 11 12 13 14 15
chain bonds :
3-10 5-7 7-8 7-9 13-19 15-16 16-17 16-18
ring bonds :
1-2 1-5 2-3 3-4 4-5 11-12 11-15 12-13 13-14 14-15
exact/norm bonds :
1-2 1-5 2-3 3-4 3-10 4-5 5-7 7-8 7-9 11-12 11-15 12-13 13-14 13-19
14-15 15-16 16-17 16-18
isolated ring systems :
containing 1 : 11 :

```

```

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:Atom
12:Atom 13:Atom 14:Atom 15:Atom 16:CLASS 17:CLASS 18:CLASS 19:CLASS
fragments assigned product role:
containing 1
fragments assigned reactant/reagent role:
containing 11
node mappings:
7:16 5:15 4:14 3:13 2:12 1:11 8:17 9:18

```

L1 STRUCTURE UPLOADED

```

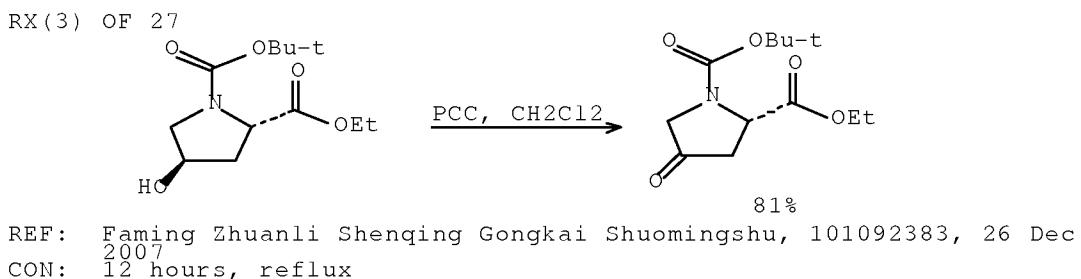
=> s 11 sss full
FULL SEARCH INITIATED 16:25:59 FILE 'CASREACT'
SCREENING COMPLETE - 26248 REACTIONS TO VERIFY FROM 1329 DOCUMENTS
100.0% DONE 26248 VERIFIED 150 HIT RXNS ( 4 INCOMP) 60 DOCS
SEARCH TIME: 00.00.02

```

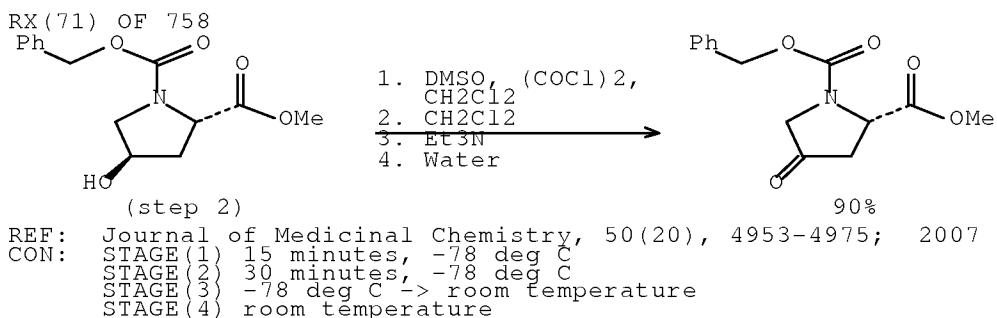
L3 60 SEA SSS FUL L1 (150 REACTIONS)

=> d tot

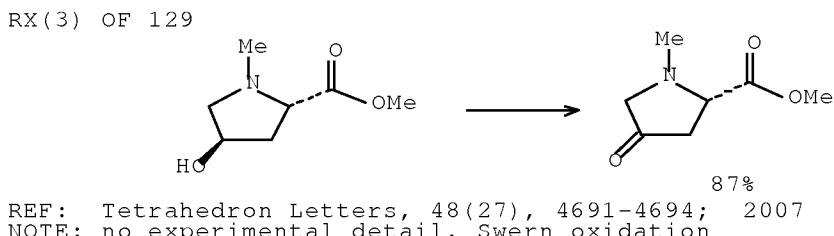
L3 ANSWER 1 OF 60 CASREACT COPYRIGHT 2008 ACS on STN



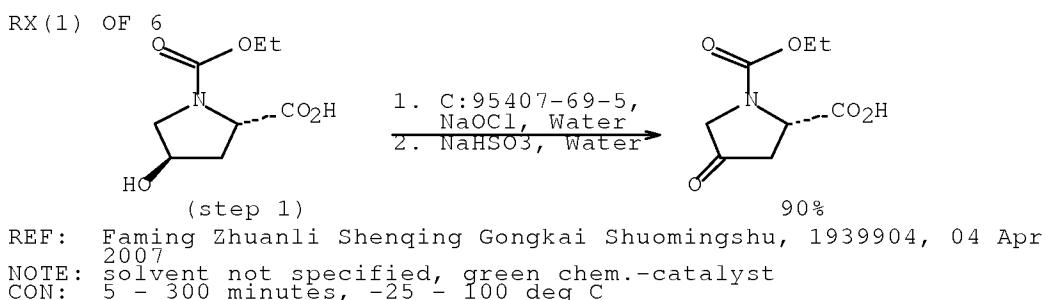
L3 ANSWER 2 OF 60 CASREACT COPYRIGHT 2008 ACS on STN



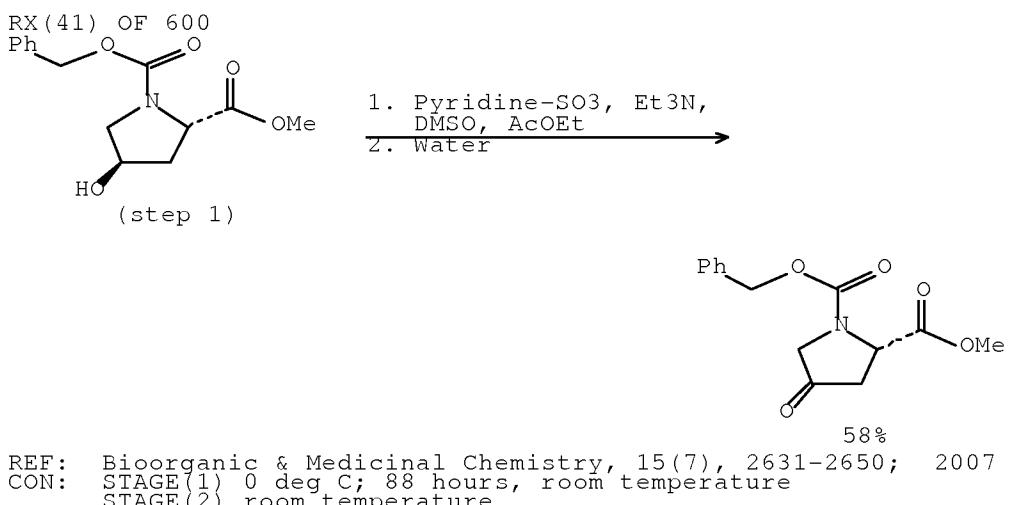
L3 ANSWER 3 OF 60 CASREACT COPYRIGHT 2008 ACS on STN



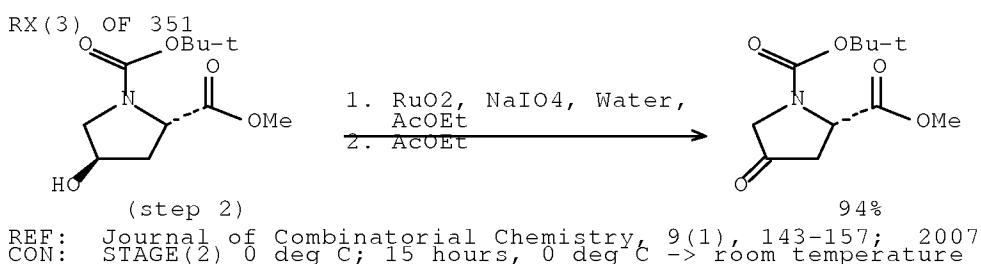
L3 ANSWER 4 OF 60 CASREACT COPYRIGHT 2008 ACS on STN

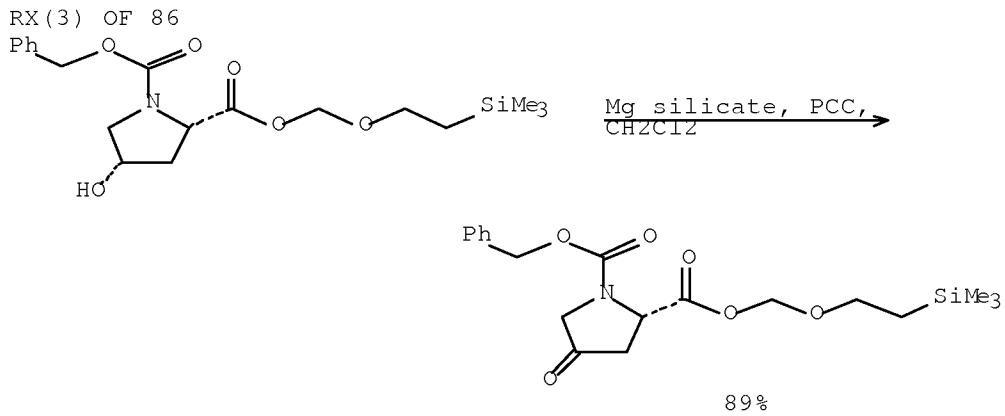


L3 ANSWER 5 OF 60 CASREACT COPYRIGHT 2008 ACS on STN

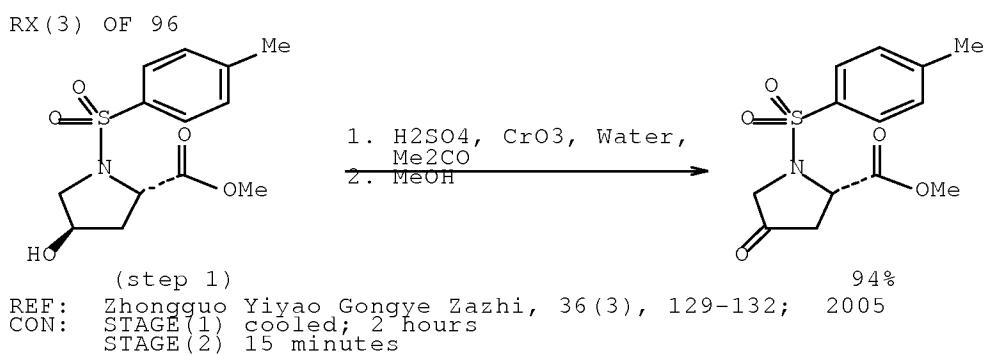


L3 ANSWER 6 OF 60 CASREACT COPYRIGHT 2008 ACS on STN

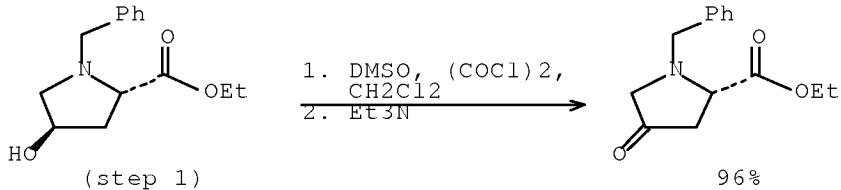




REF: Tetrahedron: Asymmetry, 17(17), 2479-2486; 2006
 NOTE: optimized on oxidation conditions, optimization study
 CON: 16 hours, room temperature



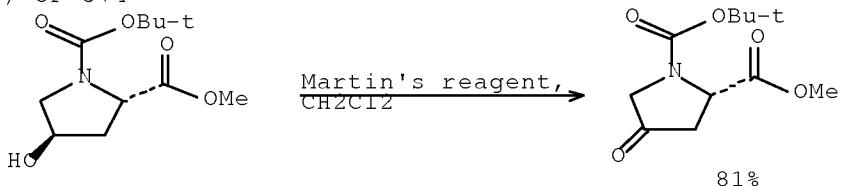
RX(5) OF 82



REF: Bioorganic & Medicinal Chemistry Letters, 16(18), 4856-4860;
2006
NOTE: Swern oxidation
CON: STAGE(1) -78 deg C
STAGE(2) -78 deg C -> room temperature

L3 ANSWER 10 OF 60 CASREACT COPYRIGHT 2008 ACS on STN

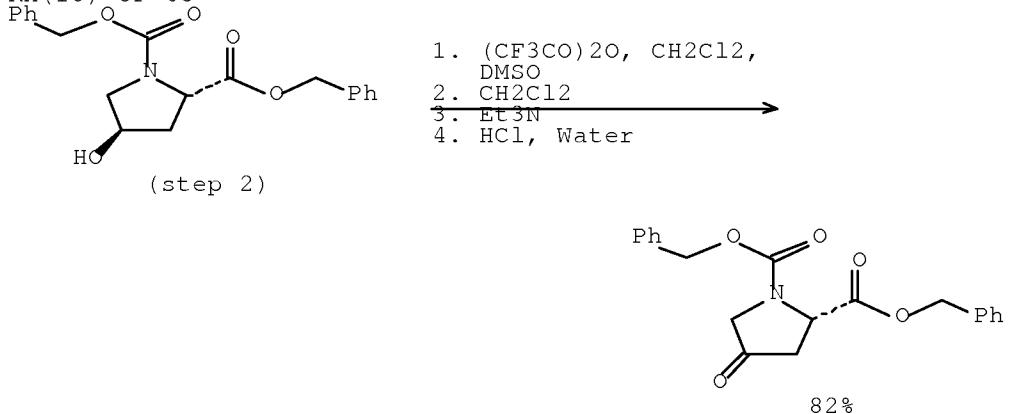
RX(24) OF 574



REF: Chemistry--A European Journal, 12(15), 4121-4143; 2006
CON: 1 hour, room temperature

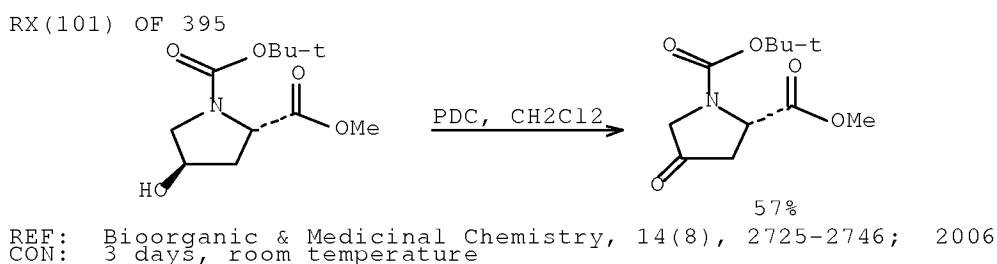
L3 ANSWER 11 OF 60 CASREACT COPYRIGHT 2008 ACS on STN

RX(18) OF 63

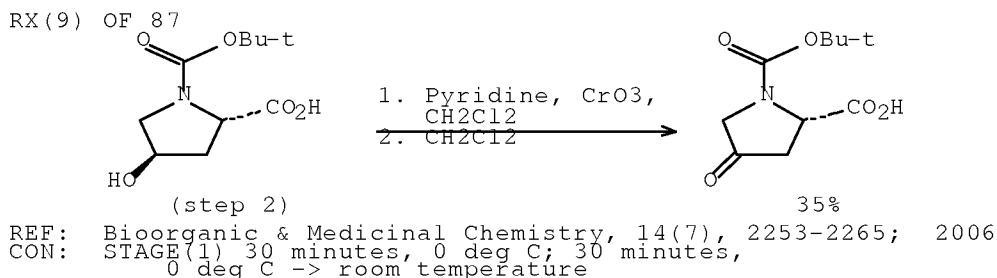


REF: Journal of Organic Chemistry, 71(13), 5004-5007; 2006
CON: STAGE(1) room temperature -> -78 deg C; 1 hour, -78 deg C
STAGE(2) 2 hours, -78 deg C
STAGE(3) -78 deg C; -78 deg C -> room temperature

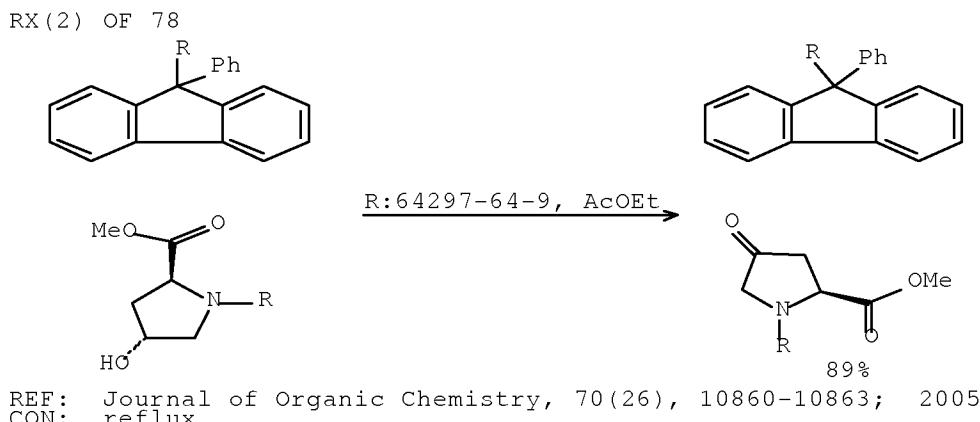
L3 ANSWER 12 OF 60 CASREACT COPYRIGHT 2008 ACS on STN



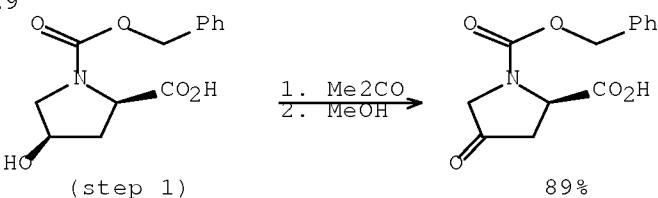
L3 ANSWER 13 OF 60 CASREACT COPYRIGHT 2008 ACS on STN



L3 ANSWER 14 OF 60 CASREACT COPYRIGHT 2008 ACS on STN



RX(3) OF 129



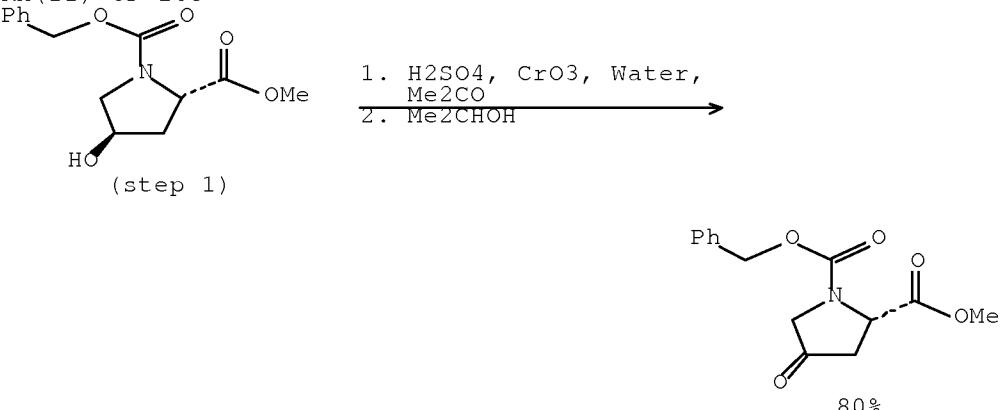
REF: Journal of Organic Chemistry, 70(22), 9002-9008; 2005

NOTE: Jones reagent used in stage 1

CON: STAGE(1) 10 minutes, room temperature; 3 hours, room temperature

STAGE(2) room temperature

RX(11) OF 265

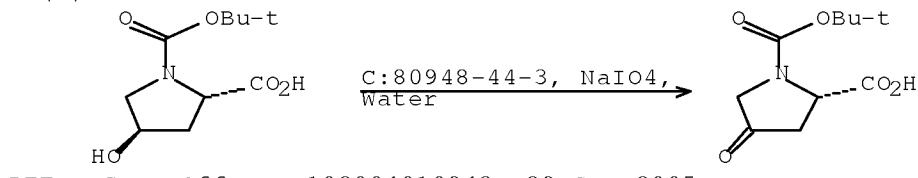


REF: Journal of Medicinal Chemistry, 48(23), 7333-7342; 2005

CON: STAGE(1) 3 minutes, room temperature; 1 hour, room temperature

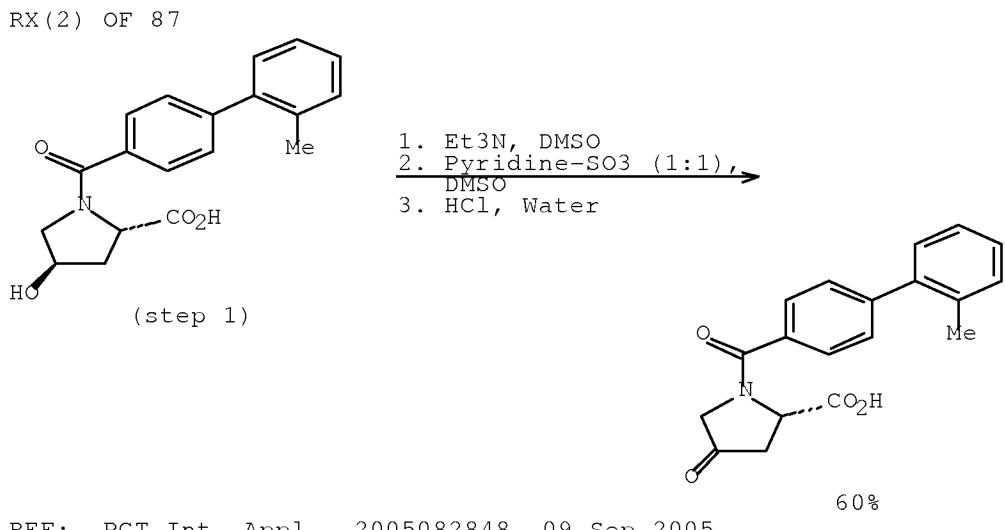
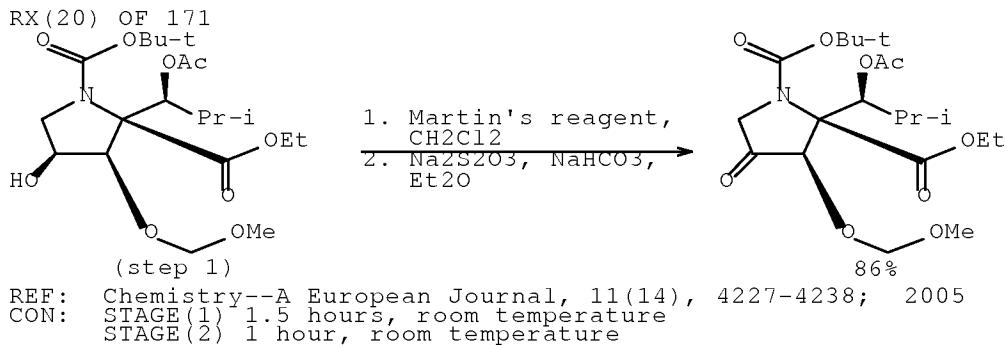
STAGE(2) 20 minutes, room temperature

RX(2) OF 3

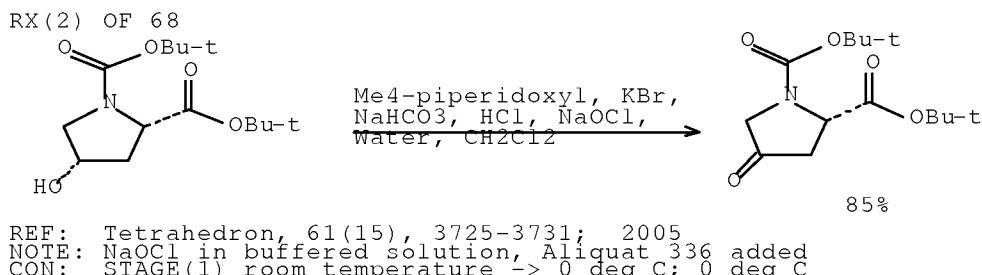
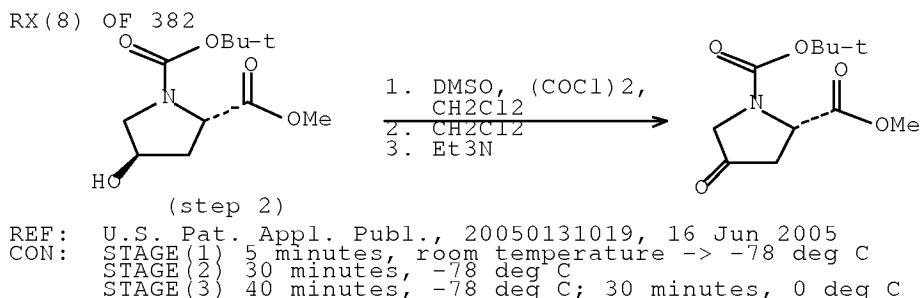
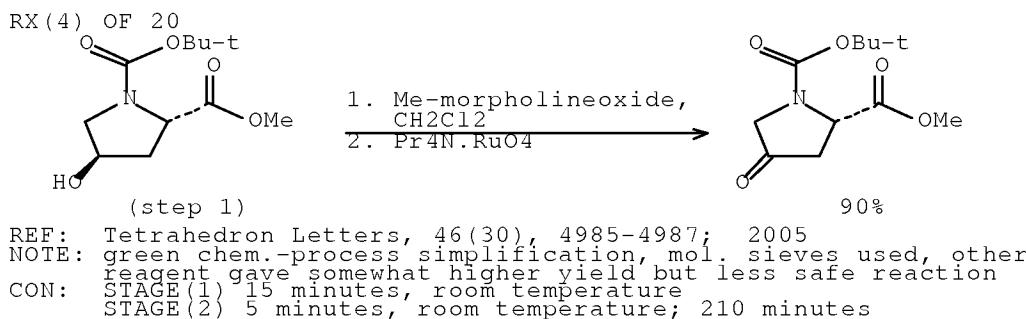


REF: Ger. Offen., 102004010943, 29 Sep 2005

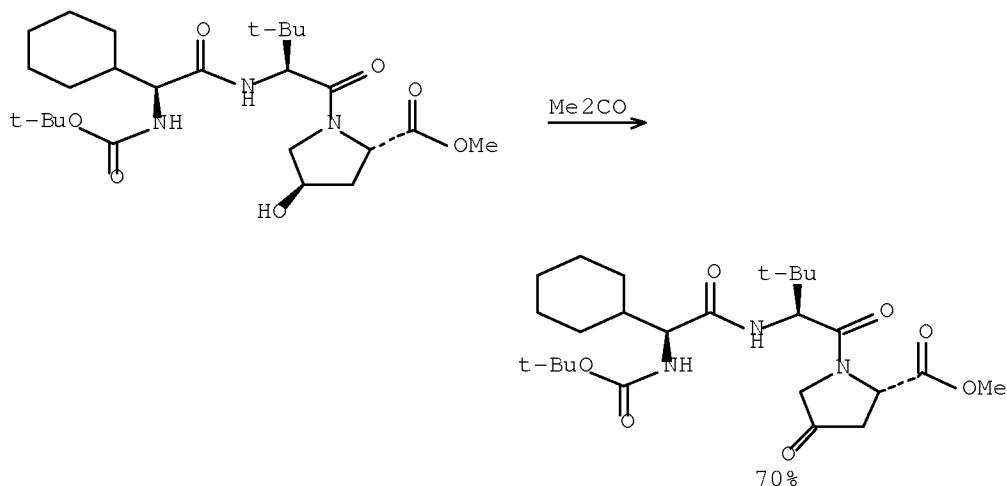
CON: STAGE(1) cooled; 1 - 1.5 hour



NOTE: workup
 CON: STAGE(1) $\frac{5}{5}$ - $\frac{20}{20}$ deg C room temperature \rightarrow 40 deg C; 40 deg C \rightarrow 10 deg C;
 STAGE(2) $\frac{5}{25}$ - $\frac{10}{10}$ minutes; 1 - 3 hour, 15 - 25 deg C;
 STAGE(3) $\frac{<30}{<30}$ deg C



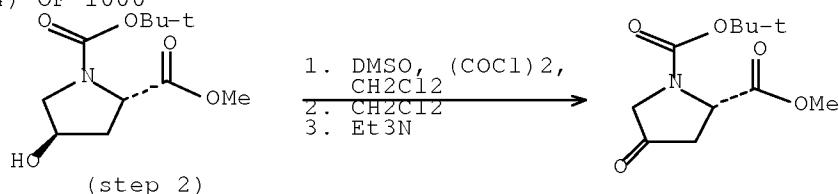
RX(5) OF 51



REF: PCT Int. Appl., 2005037860, 28 Apr 2005
NOTE: Jones reagent used

L3 ANSWER 24 OF 60 CASREACT COPYRIGHT 2008 ACS on STN

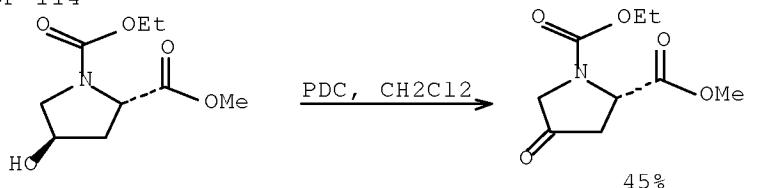
RX(94) OF 1000



REF: PCT Int. Appl., 2005023762, 17 Mar 2005
CON: STAGE(1) 5 minutes, -78 deg C
STAGE(2) 30 minutes, -78 deg C
STAGE(3) 40 minutes, -78 deg C; 30 minutes, 0 deg C

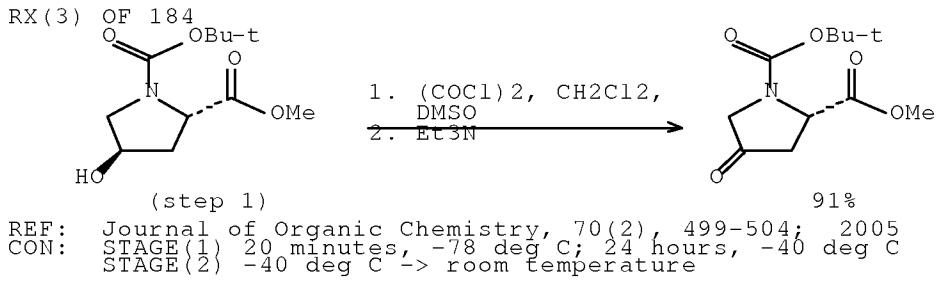
L3 ANSWER 25 OF 60 CASREACT COPYRIGHT 2008 ACS on STN

RX(55) OF 114

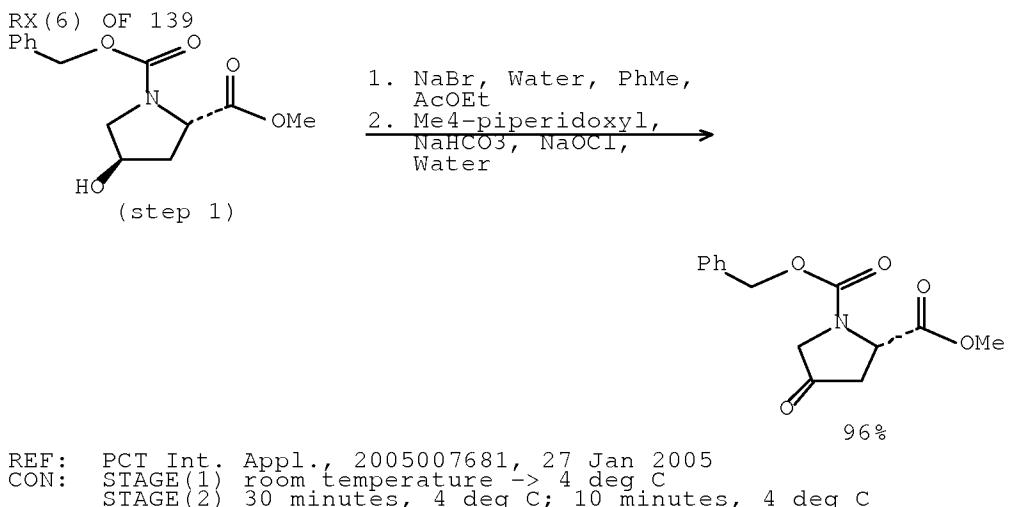


REF: Journal of Organic Chemistry, 70(3), 898-906; 2005
NOTE: celite used
CON: STAGE(1) 0 deg C; overnight, room temperature

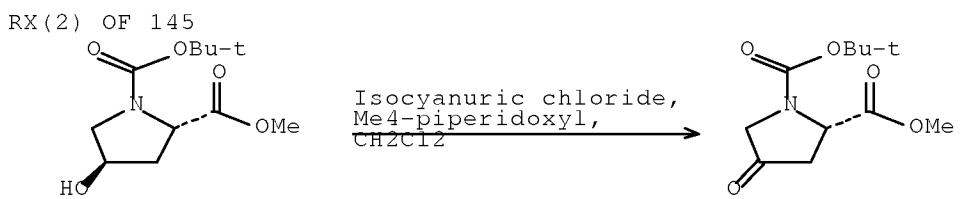
L3 ANSWER 26 OF 60 CASREACT COPYRIGHT 2008 ACS on STN



L3 ANSWER 27 OF 60 CASREACT COPYRIGHT 2008 ACS on STN

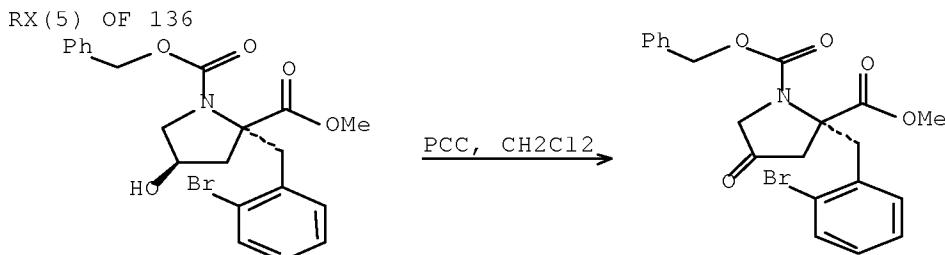


L3 ANSWER 28 OF 60 CASREACT COPYRIGHT 2008 ACS on STN



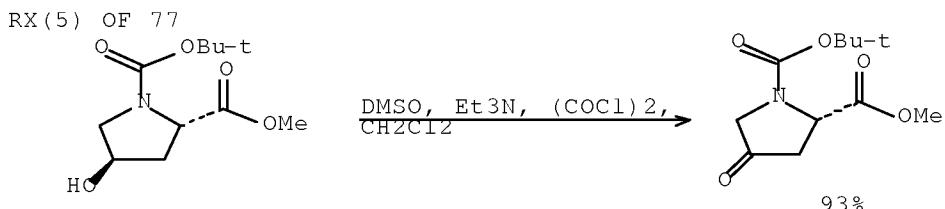
REF: Bioorganic & Medicinal Chemistry Letters, 14(22), 5699-5702;
2004
NOTE: key intermediate

L3 ANSWER 29 OF 60 CASREACT COPYRIGHT 2008 ACS on STN



REF: Tetrahedron: Asymmetry, 14(19), 3033-3041; 2003
NOTE: Florisil used
CON: 10 hours, room temperature

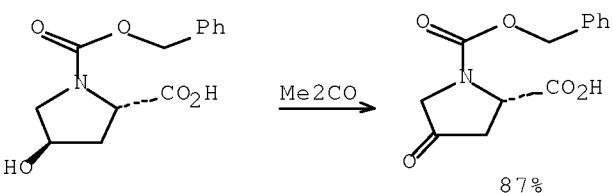
L3 ANSWER 30 OF 60 CASREACT COPYRIGHT 2008 ACS on STN



REF: Tetrahedron Letters, 44(42), 7809-7812; 2003
CON: -78 deg C

L3 ANSWER 31 OF 60 CASREACT COPYRIGHT 2008 ACS on STN

RX(2) OF 120

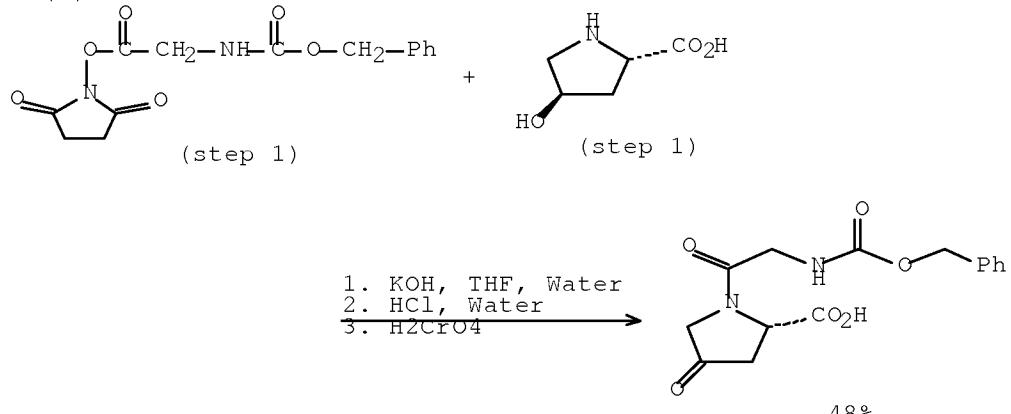


REF: Journal of the American Chemical Society, 125(16), 4702-4703; 2003

NOTE: Jones' reagent used
CON: STAGE(1) 5 minutes, 20 deg C; 30 minutes, 20 deg C

L3 ANSWER 32 OF 60 CASREACT COPYRIGHT 2008 ACS on STN

RX(2) OF 64

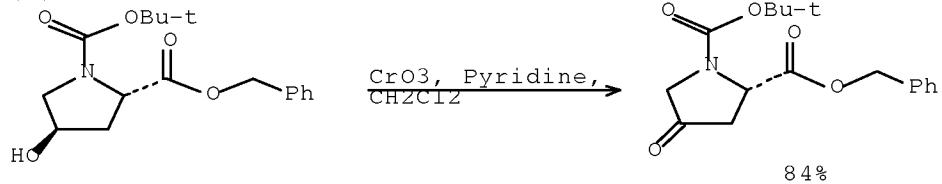


REF: Russian Journal of Bioorganic Chemistry (Translation of Bioorganicheskaya Khimiya), 28(6), 444-449; 2002

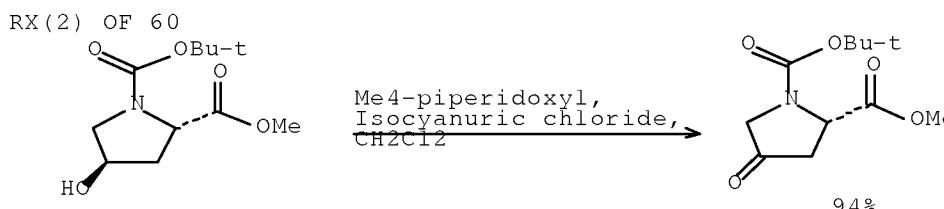
NOTE: literature prepn. stage 3
CON: STAGE(1) 2.5 hours, 20 deg C
STAGE(2) 0 deg C, pH 2 - 3

L3 ANSWER 33 OF 60 CASREACT COPYRIGHT 2008 ACS on STN

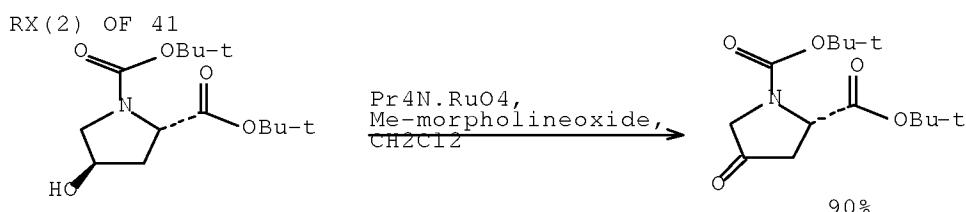
RX(3) OF 30



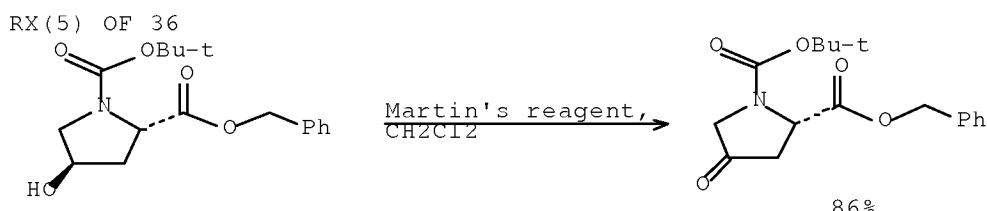
REF: Journal of Organic Chemistry, 67(20), 7162-7164; 2002



REF: Angewandte Chemie, International Edition, 41(9), 1600-1602;
2002

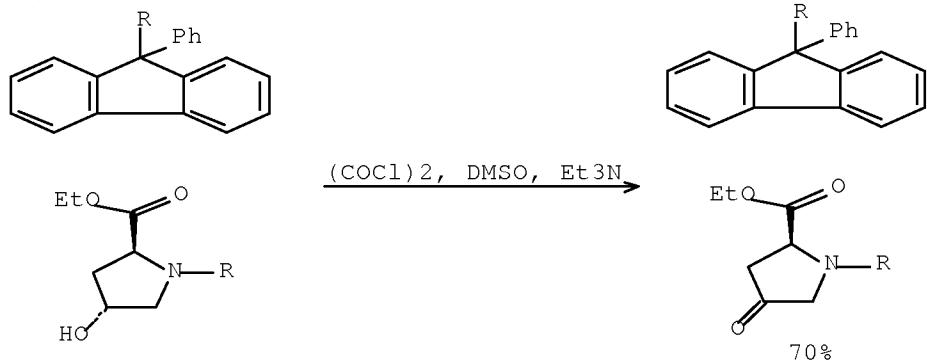


REF: Journal of Organic Chemistry, 66(10), 3593-3596; 2001
NOTE: mol. sieves used



REF: Synlett, (9), 1465-1467; 1999
NOTE: STEREOSELECTIVE

RX(2) OF 14

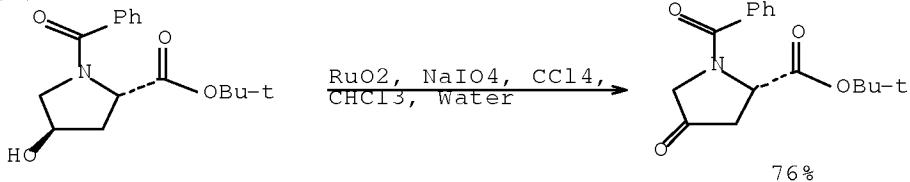


REF: Tetrahedron Letters, 38(30), 5399-5402; 1997

NOTE: literature ref.

L3 ANSWER 38 OF 60 CASREACT COPYRIGHT 2008 ACS on STN

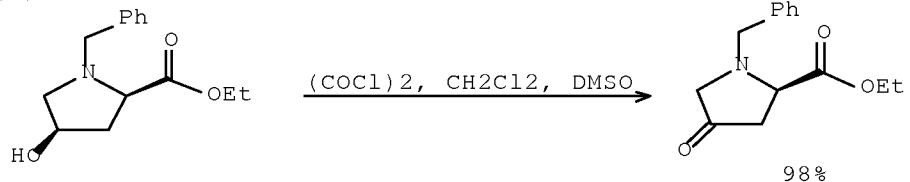
RX(4) OF 55



REF: Tetrahedron, 53(14), 5233-5254; 1997

L3 ANSWER 39 OF 60 CASREACT COPYRIGHT 2008 ACS on STN

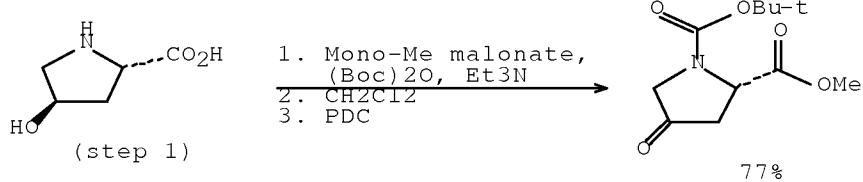
RX(2) OF 41



REF: Journal of Medicinal Chemistry, 39(15), 2990-3000; 1996

L3 ANSWER 40 OF 60 CASREACT COPYRIGHT 2008 ACS on STN

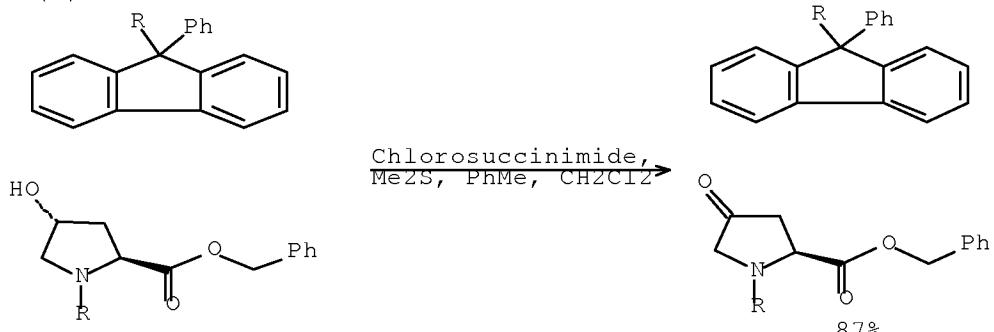
RX(1) OF 15



REF: Synlett, (1), 95-6; 1996

L3 ANSWER 41 OF 60 CASREACT COPYRIGHT 2008 ACS on STN

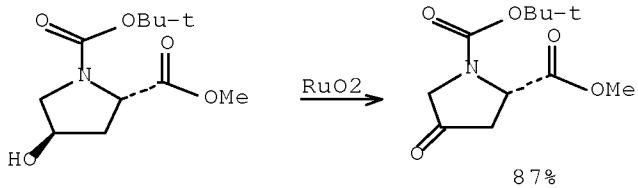
RX(2) OF 44



REF: Journal of Organic Chemistry, 61(1), 202-9; 1996

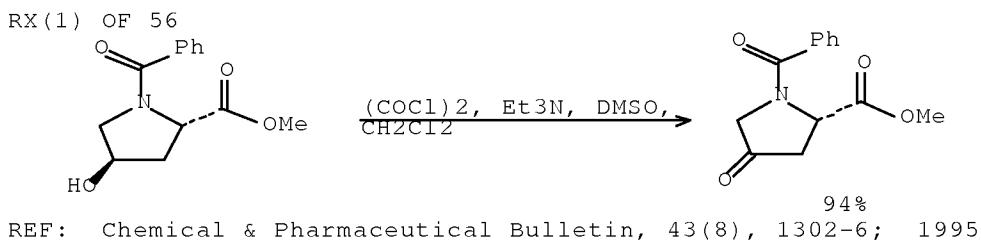
L3 ANSWER 42 OF 60 CASREACT COPYRIGHT 2008 ACS on STN

RX(3) OF 26

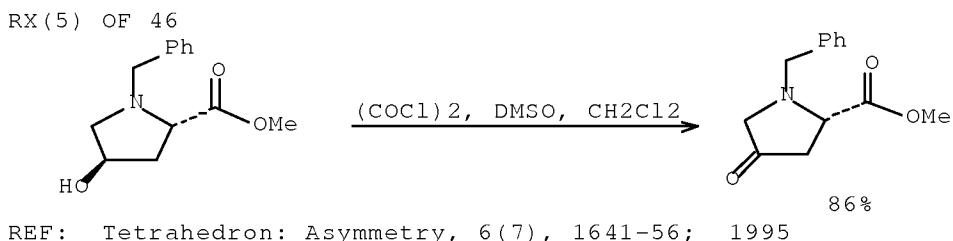


REF: Chemical & Pharmaceutical Bulletin, 43(10), 1617-20; 1995

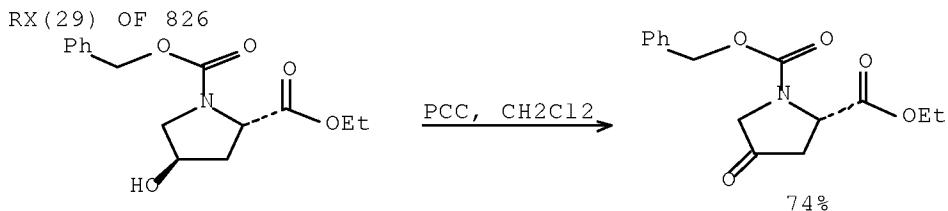
L3 ANSWER 43 OF 60 CASREACT COPYRIGHT 2008 ACS on STN



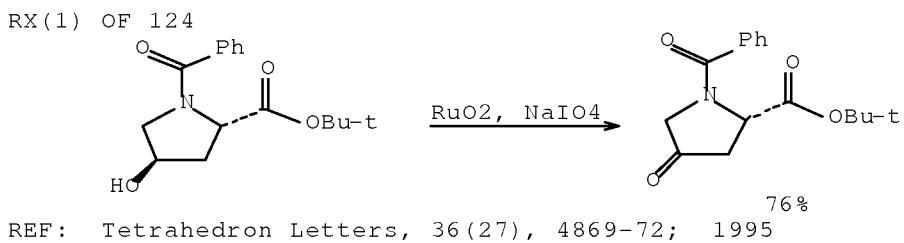
L3 ANSWER 44 OF 60 CASREACT COPYRIGHT 2008 ACS on STN



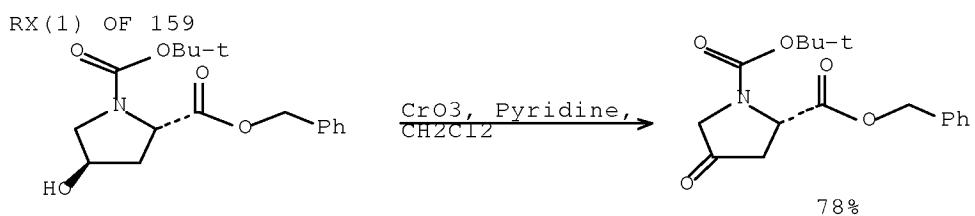
L3 ANSWER 45 OF 60 CASREACT COPYRIGHT 2008 ACS on STN



L3 ANSWER 46 OF 60 CASREACT COPYRIGHT 2008 ACS on STN

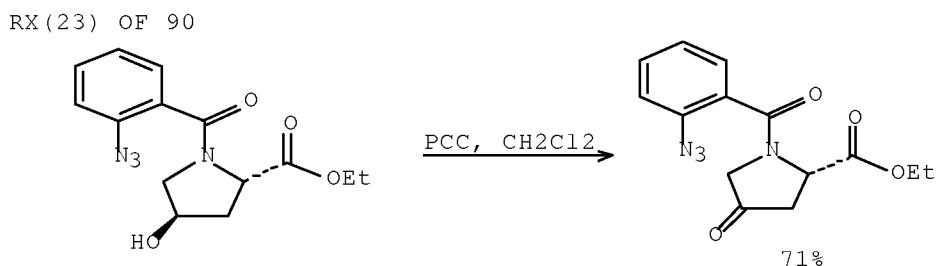


L3 ANSWER 47 OF 60 CASREACT COPYRIGHT 2008 ACS on STN



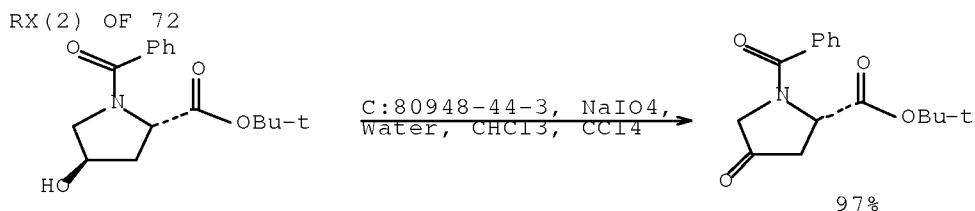
REF: Tetrahedron, 51(14), 4195-212; 1995

L3 ANSWER 48 OF 60 CASREACT COPYRIGHT 2008 ACS on STN



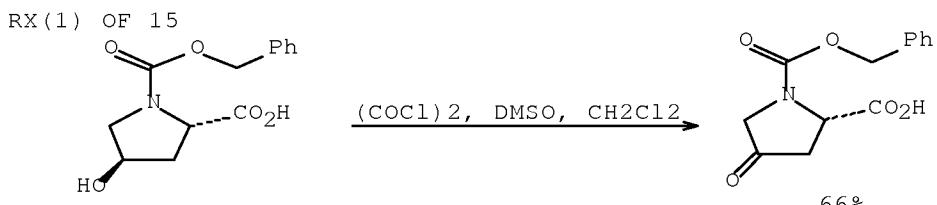
REF: Tetrahedron, 51(19), 5617-30; 1995
NOTE: product as 2:1 mixt. of syn:anti rotamers

L3 ANSWER 49 OF 60 CASREACT COPYRIGHT 2008 ACS on STN



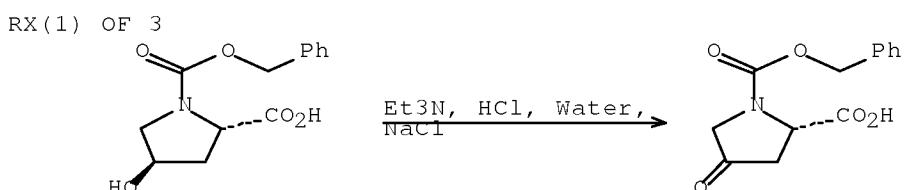
REF: Tetrahedron Letters, 35(33), 6163-6; 1994

L3 ANSWER 50 OF 60 CASREACT COPYRIGHT 2008 ACS on STN



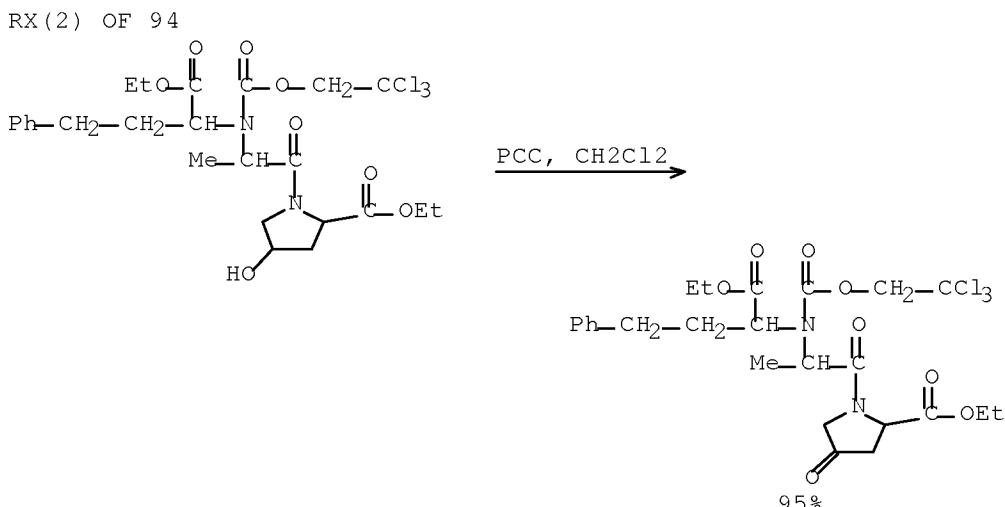
REF: Journal of Organic Chemistry, 57(19), 5264-8; 1992

L3 ANSWER 51 OF 60 CASREACT COPYRIGHT 2008 ACS on STN



REF: Ger. (East), 283626, 17 Oct 1990

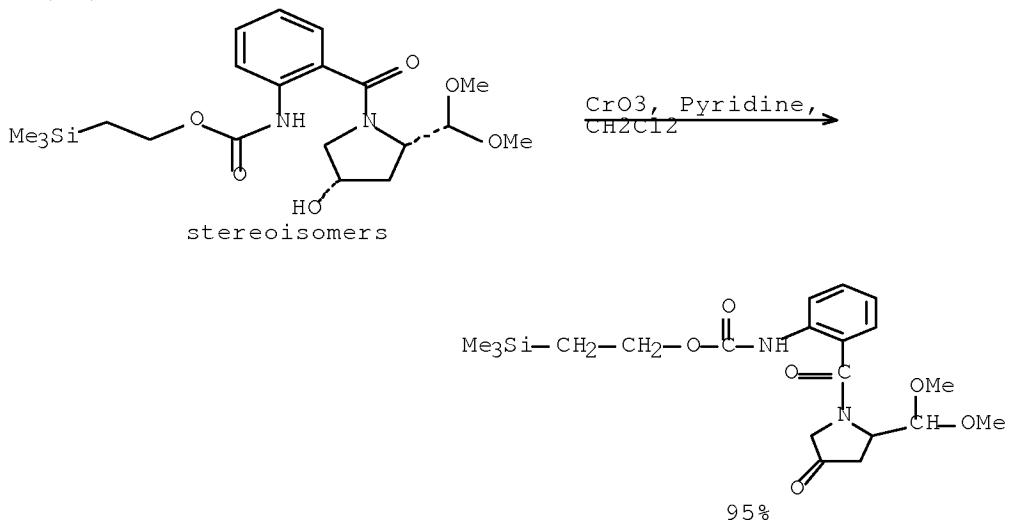
L3 ANSWER 52 OF 60 CASREACT COPYRIGHT 2008 ACS on STN



REF: Journal of Medicinal Chemistry, 33(6), 1606-15; 1990

L3 ANSWER 53 OF 60 CASREACT COPYRIGHT 2008 ACS on STN

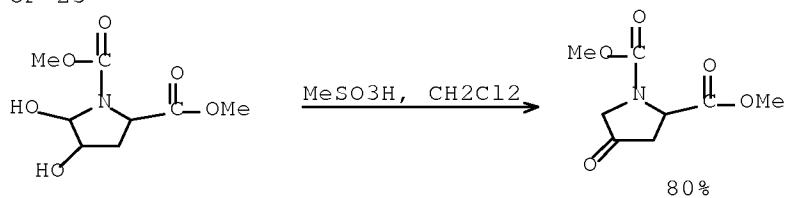
RX(29) OF 373



REF : Journal of Organic Chemistry, 54(24), 5746-58; 1989

L3 ANSWER 54 OF 60 CASREACT COPYRIGHT 2008 ACS on STN

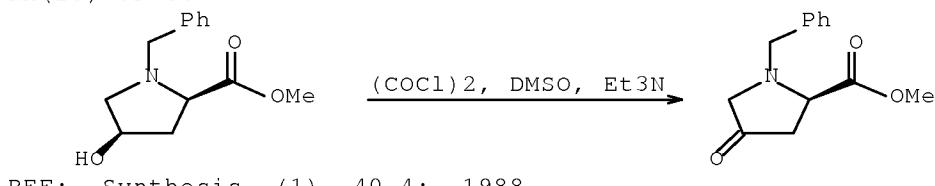
RX(11) OF 23



REF: Tetrahedron, 44(17), 5441-9; 1988

L3 ANSWER 55 OF 60 CASREACT COPYRIGHT 2008 ACS on STN

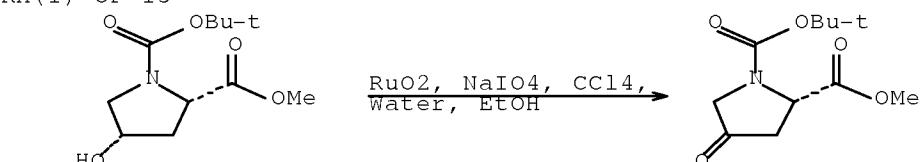
RX(13) OF 60



REF: Synthesis, (1), 40-4; 1988

L3 ANSWER 56 OF 60 CASREACT COPYRIGHT 2008 ACS on STN

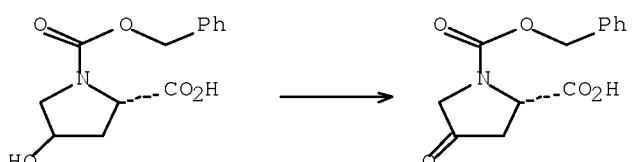
RX(1) OF 15



REF: Synthesis, (1), 81-2; 1986

L3 ANSWER 57 OF 60 CASREACT COPYRIGHT 2008 ACS on STN

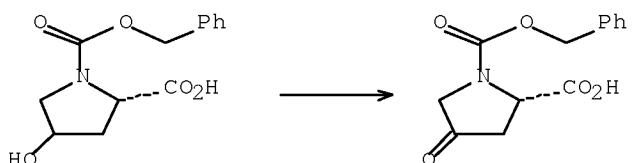
RX(2) OF 15



REF: U.S., 4311697, 19 Jan 1982

L3 ANSWER 58 OF 60 CASREACT COPYRIGHT 2008 ACS on STN

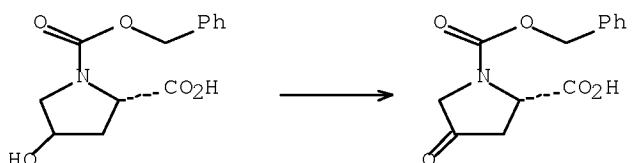
RX(1) OF 28



REF: U.S., 4296113, 20 Oct 1981

L3 ANSWER 59 OF 60 CASREACT COPYRIGHT 2008 ACS on STN

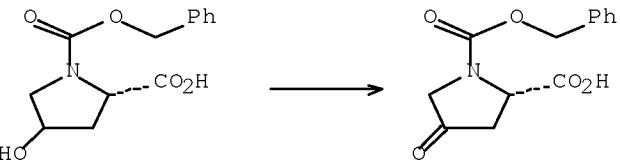
RX(2) OF 10



REF: Ger. Offen., 3009684, 24 Sep 1981

L3 ANSWER 60 OF 60 CASREACT COPYRIGHT 2008 ACS on STN

RX(1) OF 9



REF: Belg., 882366, 22 Sep 1980

=> log hold

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

FULL ESTIMATED COST

ENTRY

SESSION

178.06

297.39

SESSION WILL BE HELD FOR 120 MINUTES

STN INTERNATIONAL SESSION SUSPENDED AT 16:29:54 ON 14 APR 2008